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DEVELOPMENT OF Si/SiGe HETEROSTRUCTURES

R.J. Hauenstein and O.J. Marsh

Hughes Research Laboratories

3011 Malibu Canyon Road

Malibu, California 90265

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QUARTERLY REPORT

$Si_{1-x}Ge_x$ CONTRACT

I. Introduction

With the recent advances in Si molecular beam epitaxy (MBE), a heterojunction-based device technology for Si may soon be at hand. Strained-layer $Si_{1-x}Ge_x$ epitaxial alloy films and coherently strained $Si_{1-x}Ge_x$/Si multilayer structures have been grown very successfully by MBE. $Si_{1-x}Ge_x$/Si systems are of considerable interest because they promise to extend the capabilities of heterojunction-based devices to the already well established realm of Si technology. The major impact of a heterojunction technology applied to Si electronic devices is expected to be twofold: in the performance improvement of certain **conventional** Si devices such as the n-p-n bipolar transistor, and in the development within Si technology of **novel** device structures such as the High Electron-Mobility Transistor (HEMT). For the n-p-n bipolar transistor, replacement of the base with a p-type $Si_{1-x}Ge_x$ alloy layer to form the heterojunction bipolar transistor (HBT) is expected to result in higher speed and higher frequency (40 GHz) operation than is offered by the conventional bipolar transistor (20 GHz). This is because of the large (~100 meV) negative valence band offset ($\Delta E_v \equiv E_v^{Si} - E_v^{SiGe}$) at the emitter-base junction. The resultant large potential barrier presented to holes would allow for a heavier base-layer and a lighter emitter-layer dopant concentration while maintaining the large base-emitter electron/hole injection ratio needed for high current gain. Improved frequency performance is then possible because of the reduced series resistance in the more heavily doped base layer, and also a reduced base-emitter capacitance as the emitter need not be as heavily doped, both improvements leading to a reduced RC time constant. For the HEMT, high speed operation is obtained through the enhancement of electron mobility which occurs due to two-dimensional carrier confinement (using the conduction band offset) to a thin sheet adjacent to the interface. This electron sheet is spatially segregated from the donors, resulting in improved mobility through reduced ionized-impurity scattering. Thus, in both the HBT and the HEMT, the physical properties of the $Si_{1-x}Ge_x$/Si heterojunction are exploited to achieve something that is not possible in either material alone, and, in contrast with other materials systems, $Si_{1-x}Ge_x$/Si heterojunction-based device structures are compatible with a mature and extensive Si device processing technology.

In electronic devices based on $Si_{1-x}Ge_x$/Si heterostructures, the physical and materials concerns of greatest importance are the following: (1) the "bulk" band structures of individual layers, (2) the band offsets between layers, (3) the structural quality of layers and interfaces, (4) the control of compositional and dopant profiles, and (5) the effects of strain. In **any** heteroepitaxial materials system, the first four of these items must be controlled, or at least understood, in order to successfully produce device structures. However, because of the large (4.2%) lattice constant mismatch between Si and Ge, strain plays a particularly important role in the $Si_{1-x}Ge_x$/Si system, a role much more critical here than in lattice-matched systems such as GaAs/AlAs. The lattice mismatch at a $Si_{1-x}Ge_x$/Si interface must be accommodated in one of two ways (or a combination thereof): through the formation of misfit dislocations, or through elastic distortion (strain). The particular mode of misfit accommodation can be expected to significantly alter device performance as we now discuss.

Interfacial dislocations at heterojunction interfaces are generally undesirable as they give rise to leakage currents in devices depending on charge transport across the junction (such as the HBT), and result in a mobility reduction in HEMT-like device structures. On the other hand, elastic strain modifies both bandstructure and band offset. For example, the **sign** of the $Si_{1-x}Ge_x$/Si conduction band offset ΔE_c is strain-dependent for certain compositions while ΔE_v is always of the same sign, making possible both type-I and type-II band alignments. Also, strain effects can remove energy degeneracies among conduction or valence band extrema.

These strain effects may be exploited. For instance, in the ideal HBT structure grown on (100)-Si, assuming a Si-like conduction band structure with six equivalent Δ-line minima (valid for compositions $x<0.85$), the coherent base-layer strain (an in-plane biaxial compression accompanied by an extension along the interface normal) raises the energy of the two minima aligned along the interface normal while lowering that of the other four minima. This results in a lower effective mass component for transport normal to the interface, and the partial removal of intervalley phonon scattering, both of which enhance the electron mobility across the heterojunction. Another example concerns the HEMT structure coherently strained to a thick $Si_{1-x}Ge_x$ buffer-layer lattice constant. In this case ΔE_c can be made negative, resulting in two-dimensional electron confinement on the Si rather than the $Si_{1-x}Ge_x$ side of the interface, thereby eliminating alloy scattering mechanisms. In addition, the strain in this case is opposite to that described above for the HBT, resulting this time in an **in-plane** electron mobility enhancement in the HEMT (for similar reasons to those cited above for the HBT). Clearly, strain plays an important role in determining the electronic properties of $Si_{1-x}Ge_x$/Si heteroepitaxial structures.

II. Device Goals

In this contract we have focused our attention on $Si_{1-x}Ge_x$ electronic devices and have sought to target those specific device structures which we believe show the greatest potential for success. We have identified the following target device structures: the HEMT, the High Hole-Mobility Transistor (HHMT), the p-n heterojunction diode (HD), and ultimately the HBT. In our proposal we proposed to fabricate working unipolar (HEMT and HHMT) and bipolar (HD) devices. $Si_{1-x}Ge_x$/Si HEMT structures have already been grown by MBE and successful devices demonstrated at AEG in Germany. The development of a HHMT device would provide a valuable complementary logic capability to HEMT-like unipolar devices. For bipolar devices, future development of devices such as the HBT will be necessarily based on an understanding of the single-heterojunction diode. Therefore, it is appropriate to study the HD in detail before attempting more elaborate bipolar device structures. Finally, based on our results for the HD, we wish to make a serious attempt at the HBT though detailed development of this device will take place under our own IR&D projects.

III. Methods and Capabilities

At HRL, we have a number of facilities available for the fabrication and characterization of MBE-grown $Si_{1-x}Ge_x$ heteroepitaxial layers. Our new Perkin-Elmer Si MBE system is expected to be in place by Feb 1988. This system will have the capability of codeposition of Si and Ge onto 3-in. heated substrates, with codoping capability from both conventional effusion and low-energy ion sources. In situ physical characterizations include reflection high-energy electron diffraction (RHEED) and Auger analysis capabilities. Important ex situ materials characterizations available at HRL include secondary ion mass spectroscopy (SIMS), scanning electron microscopy (SEM), differential-interference contrast (Nomarski) optical microscopy, and a complete x-ray laboratory. In particular, we have recently (under a related IR&D project) acquired a four-crystal x-ray monochromator (Bartels) for the purpose of characterizing our MBE-grown $Si_{1-x}Ge_x$ epilayers. In addition, our group is particularly well equipped to make electrical and optical characterizations of as-grown materials. We currently perform photoluminescence (PL) (using both conventional and Fourier-transform spectroscopy) and temperature-dependent Hall effect and resisitivity measurements on a routine basis, and have also recently acquired an electrochemical C-V profiler (Polaron) in order to characterize dopant profiles in our $Si_{1-x}Ge_x$ films. In addition, our well-equipped optical laboratory permits us to set up other (electro)optical measurements such as Raman spectroscopy and photoresponse quite readily.

We have made arrangements for access to needed characterization tools which are not directly available at HRL. In particular, transverse electron microscopy (TEM), including both plan-view and cross-sectional imaging as well as high-resolution lattice-imaging capabilities. is expected to be done collaboratively with the materials research group at Caltech. Rutherford backscattering spectroscopy (RBS) is another vital research tool in this type of work. For this. HRL has access to equipment at Cal State Los Angeles although at present this equipment is capable of acquiring unchanneled (random) spectra only. Finally. we plan on making use of commercial services. particularly for spreading-resistance measurements. and also RBS channeling. as required.

In fabricating HEMT and HD structures we plan to use our low-temperature ($\leq 350^{\circ}$ C) plasma silicon oxide deposition system for photolithographic patterning with reactive ion etching. Contacts to these structures will be formed by ion implantation and thermal. rapid thermal. or pulsed-UV annealing processes. Metalizations will be performed by electron beam evaporation.

In addition to experimental methods listed above. we also have theoretical efforts (under concurrent contract and IR&D programs) being set up to investigate electronic bandstructure and strain effects in $Si_{1-x}Ge_x$/Si heteroepitaxial structures. as well as device modeling. and the low-energy ion-implantation doping process for MBE. This theoretical work will take place both at HRL and Texas A&M as part of a joint program.

QUARTERLY REPORT

$Si_{1-x}Ge_x$ CONTRACT

IV. Approach

Our approach can be summarized as follows: (1) solve the materials (structural) problems. (2) get doping under control. (3) evaluate electrical transport properties on pre-device test structures. (4) fabricate and test device structures. and (5) optimize device performance. Our efforts under this work will be to identify and establish the process parameters necessary to produce HEMT. HHMT. and HD devices. and to demonstrate a working HBT. However. we will not attempt to optimize the HBT under this program. Under a parallel IR&D project. our research will be directed more toward a fundamental understanding of the relevant physical processes involved in the MBE growth. doping. subsequent processing. device operation. and also HBT optimization. When it is relevant we will identify and report here results obtained under the IR&D project.

Our first task is to address the materials issues involved in achieving the desired device structures. This will involve detailed **structural** and **compositional** characterization of epitaxial films with the use of RHEED. x-ray. TEM. SEM and Nomarski. defect-etch. and RBS methods. The effort here will be on obtaining defect-free materials. physically abrupt interfaces. and coherently strained epitaxial structures. MBE growth techniques will be developed. and the optimum growth conditions. most notably. substrate temperature and deposition rate. will be determined.

QUARTERLY REPORT

$Si_{1-x}Ge_x$ CONTRACT

The next task concerns the control of dopant concentration profile, and identification and characterization of doping from unintentional sources. For the HEMT and HHMT, the major concern is the position of the "delta-doping" spike relative to the heterojunction; for the HD structure, the electrical abruptness, position, and concentrations of the p-n doping junction relative to the compositional heterojunction are the main issues. The identity of dopants is expected to be accomplished with PL and possibly SIMS, and the dopant profiles evaluated through the use of SIMS, spreading resistance and electrochemical C-V profiling techniques.

Once structural and doping issues are under control, electrical transport measurements on predevice diagnostic structures can be attempted. In particular, we plan to make temperature-dependent Hall effect and resistivity measurements in preliminary HEMT and HHMT structures to assess carrier scattering mechanisms. For the HD, evidence of bulk and interfacial deep level traps will be sought through I-V and (frequency-dependent) C-V measurements, and possibly, through deep level transient spectroscopy (DLTS) as well. Fundamental issues like the magnitude of band offsets will be studied concurrently under IR&D projects. At this point, we will be in a position to begin fabrication of the actual device structures. The device parameters will be measured and studied as a function of growth conditions. This information will allow iteration toward optimum performance. Finally, the device capabilities will be demonstrated in some simple test circuits.

V. Progress (Sep thru Dec 1987)

During the interim between the start of this contract and the arrival of our Si MBE equipment, we have begun work on our above agenda through a collaborative effort involving Perkin-Elmer and Caltech. The progress that we wish to report here concerns materials (structural) issues: specifically, the investigation of misfit accommodation in various lattice-mismatched $Si_{1-x}Ge_x$/Si epitaxial structures grown on Si substrates. Our emphasis is on establishing the growth conditions required to produce coherently strained (dislocation-free) films. This effort parallels an IR&D-related joint project with the same collaborators to investigate the kinetics of misfit accommodation in these same structures. Under our IR&D project, we have been studying strain relaxation phenomena in strained-layer $Si_{1-x}Ge_x$/Si superlattices. In that work, our most significant finding thus far has been the observation that the growth temperature has a strong effect upon the degree of coherent strain within the $Si_{1-x}Ge_x$ layers of the superlattices. In particular, we have found that at lower growth temperatures ($\simeq$365°C) the superlattices exhibit nearly full coherent strain, and that between this temperature and 530°C the $Si_{1-x}Ge_x$ layers relax significantly toward their bulk lattice constant value. However, in that work, the overall crystalline quality of the films, especially, threading dislocation and stacking fault densities, have not been extensively studied at this time, and these structural defects may be found to be minimized at higher growth temperatures than 365°C (or through post-growth annealing procedures). Moreover, the results are strictly valid only for the superlattice structures that were studied, and may vary for different multilayer configurations. Hence, more detailed work is needed, and in particular, we cannot yet conclude that the temperature which results in maximum coherent strain in $Si_{1-x}Ge_x$/Si superlattices is necessarily the optimum temperature for growth of our HEMT, HHMT, HD, and HBT device structures.

To better characterize strain and crystalline quality in our epitaxial films, we have recently acquired a four-crystal x-ray monochromator as mentioned above. This instrument accomplishes monochromation of Cu K_α radiation ($\Delta\lambda/\lambda=2.3X10^{-5}$) through successive Bragg reflection off of four Ge crystals. In our monochromator, either the (220) or the (440) Bragg reflections can be selected, permitting a tradeoff between angular beam divergence (down to 5 arc sec) and beam intensity. This high resolution capability will greatly facilitate characterization of crystalline quality through analysis of the FWHM of diffraction peaks as well as precise lattice constant and strain determinations from peak positions. In addition to the monochromator, we have purchased the necessary hardware to allow automated data acquisition of x-ray scans in a θ-2θ geometry. This hardware includes a stepper motor drive system, and an IBM personal computer with the necessary interface cards. Meanwhile, we are in the process of testing the monochromator itself while awaiting delivery of the remainder of our equipment.

At present, we are attempting to determine the growth parameters needed for the fabrication of highly abrupt, planar, and coherent interfaces. For this purpose, we have requested Perkin-Elmer to provide us with a matrix of $Si/Si_{1-x}Ge_x/Si$ HBT-like structures, with x values of 15% and 30%, and alloy layer thicknesses of approximately 1500 and 3000 Å. We note here that the HBT structure is simpler to grow and characterize than the HEMT or HHMT, and in terms of interfacial and crystalline quality, may in fact prove to be **structurally** appropriate for the HD as well since the strained $Si_{1-x}Ge_x$ must not exceed the critical thickness if the heterojunction is to be free of misfit dislocations. The alloy layers of these samples are to be grown initially near 365 °C (based on our IR&D studies of coherent $Si_{1-x}Ge_x/Si$ strained-layer superlattices), and at thicknesses and compositions which have been chosen to straddle the critical thickness data of Bean et al. for $Si_{1-x}Ge_x$ alloy films. In order to facilitate interfacial abruptness, the deposition rates near the $Si/Si_{1-x}Ge_x$ and $Si_{1-x}Ge_x/Si$ interfaces are to be slowed as well. We have received the first of these samples from Perkin-Elmer, and have submitted specimens to our Caltech collaborator (Dr. C.W. Nieh) for TEM plan view and cross-sectional analyses.

VI. Present Status

The present status of our facilities is as follows. Our Si MBE system is scheduled for delivery by Feb 1988. Ours will be the first delivery of the new Perkin-Elmer Si MBE system. At Perkin-Elmer, assembly of our MBE system is complete, and initial performance testing and evaluation has begun. Meanwhile, our laboratory facilities are being readied for the arrival of the new MBE equipment. The facilities setup is expected to be completed by the end of Jan 1988, coincident with the arrival of the MBE machine. Also, we have arranged for TEM characterization of our materials through collaboration with members of Caltech's materials research group. Most other important characterizations already exist at HRL and are available to us. Finally, we have identified the important fabrication processes and will implement them for device structure fabrication.

VII. Summary

In summary, during the past quarter we have targeted our device objectives under this contract, identified the relevant device issues, assembled the required analytical tools,

QUARTERLY REPORT

$Si_{1-x}Ge_x$ CONTRACT

detailed our research approach toward these device objectives, and lastly, established an interim collaboration and begun work on the materials aspects of $Si_{1-x}Ge_x/Si$ epitaxial heterostructure devices until the arrival of our Si MBE system. We have no specific technical results of this research to report at this time under this contract; however, on a parallel, internally sponsored $Si_{1-x}Ge_x$ research project with the same collaborators, we have identified the significance of growth temperature in determining the degree of coherent strain in strained-layer $Si_{1-x}Ge_x/Si$ superlattices. Under the present contract, we have begun (with our collaborators) to produce and characterize a matrix of samples having an HBT device structural configuration, making use of information obtained under our internal research efforts. The purpose of these samples is to establish the growth conditions needed to produce coherently strained $Si_{1-x}Ge_x/Si$ heteroepitaxial device structures on Si with optimum materials quality.